

Nucleation in two dimensional Ising system: Classical theory and computer simulation

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Abstract: We have studied the nucleation in the two dimensional Ising model by Monte Carlo simulation. The nucleation time has been studied as a function of the magnetic field for various system sizes. The logarithm of the nucleation time is found to be proportional to the inverse of the magnetic field. The crossover field and time are studied as a function of system size. The observed variations are consistent with the prediction of classical nucleation theory.

Keywords: Ising model, Nucleation, Monte Carlo simulation
PACS Numbers: 05.50 +q

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I. Introduction

The dynamical aspects of Ising model is an active area of modern research. How does the magnetisation relax towards its equilibrium value, if we start the dynamics with all spins parallel ? How long is the lifetime of a metastable state if a magnetic field is antiparallel to the initial spin orientation ? Can one answer all these questions in the light of growing and shrinking droplets ?

What happens if all spins are up in presence of a small opposite magnetic field and the system is below its critical temperature (T_c) ? The magnetisation first settles to a metastable state, and then a droplet larger than a critical size is formed. As the time passes, this droplet grows radially and the magnetisation jumps to a negative value. Classical nucleation theory (CNT) [1] predicts that the logarithm of the nucleation rate (number of supercritical droplets formed per unit time per unit volume) to be asymptotically proportional to h^{1-d} in d dimension, where h is the normalized magnetic field. This has been verified in the three dimensional Ising model by Monte Carlo simulation [2]. There are some difficulties in measuring the nucleation rates by checking how long the magnetisation takes to leave its metastable value. In the asymptotic limit of field (h) going to zero for a finite lattice size, only one supercritical droplet will be formed and it grows to cover the whole lattice. This is the proper nucleation regime and the nucleation rate is the reciprocal of the product of nucleation time and lattice volume. On the other hand, in the coalescence regime, with the lattice size going to infinity at fixed field (h), many such supercritical droplets will be formed at a time and they grow and coalesce and as a consequence the magnetisation switches sign. This effect, already discussed by Binder and Müller-Krumbhaar [3] and mathematically shown by Schonmann [4], was demonstrated by Ray and Wang [5] for Swendsen-Wang dynamics.

In this paper, we have studied the nucleation in two dimensional Ising system by Monte Carlo simulation with heat-bath dynamics. We have also studied the system size dependent crossover (from nucleation regime to coalescence regime) and compared the simulational results with the results of classical nucleation theory.

II. Classical nucleation theory

We review briefly the results of classical nucleation theory far below T_c . The equilibrium number (per site) n_s of droplets, containing s spins is

$$n_s \sim \exp(-F_s/KT)$$

where F_s is the formation free energy of the droplet of size s and K is the Boltzmann constant. CNT assumes a spherical droplet shape and takes

$$F_s/KT = -hs + 2\pi^{1/2}s^{1/2}\sigma$$

where σ is the surface tension. The critical size s^* of a droplet which maximises the free energy, is

$$s^* = \pi\sigma^2/h^2$$

and

$$F_{max} = \pi\sigma^2/h.$$

The number n_{s^*} of droplets having the critical size is

$$n_{s^*} \sim \exp(-F_{max}/KT) \sim \exp(-\pi\sigma^2/hKT).$$

The nucleation rate (J) is proportional to n_{s^*}

$$J \sim n_{s^*} \sim \exp(-\pi\sigma^2/hKT).$$

In the nucleation regime, the nucleation time τ is inversely proportional to the nucleation rate J ,

$$\tau \sim J^{-1} \sim \exp(\pi\sigma^2/hKT). \quad (1)$$

In the coalescence regime, the number of spins in a supercritical droplet will grow as t^d ($d = 2$ here). For a steady rate of nucleation, the rate of change of magnetisation is Jt^d , for a fixed change (Δm) in magnetisation during the nucleation time τ ,

$$\Delta m \sim \int_0^\tau Jt^d dt \sim (J\tau)^{d+1}.$$

So, in the coalescence regime,

$$\tau \sim J^{-1/(d+1)} \sim \exp(\pi\sigma^2/3hKT). \quad (2)$$

III. Numerical Results

We have considered a square lattice (of linear size L) with nearest neighbour ferromagnetic interaction. Initially, all spins are taken parallel (up) and used the heat-bath dynamics to simulate the nucleation phenomena. We have now allowed the system to relax to another equilibrium state via a metastable state in presence of an opposite (negative) magnetic field at a temperature ($t = J/KT = 5/8$) below the critical temperature ($J/KT_c = 0.440687$). We have used helical boundary condition in one direction and periodic boundary condition in the other direction.

In the nucleation regime, the true nucleation time is quite large and fluctuates enormously. Here, we define the nucleation time as the time required by the system to have the magnetisation below 0.9. This choice is quite arbitrary and the results do not depend considerably on the choice of this threshold. The range of temperature has been chosen in such a way that the metastable values, at those temperatures,

always lie above 0.9. Due to the huge fluctuations in the nucleation time, to avoid the waste of computational time we have taken the *median* nucleation time instead of taking the (algebraic) mean.

Figure 1 shows the plot of nucleation time (at a fixed temperature, $J/KT = 5/8$) versus the normalized magnetisation h for different system sizes. It shows clearly the crossover from a nucleation regime (small lattices, smaller fields, long nucleation time) due to a single supercritical droplet to a coalescence regime with many such supercritical droplets (large lattices, larger fields, short nucleation time). The larger the lattice is, the longer is the nucleation time above which the proper nucleation regime can be found. So, by taking a smaller lattice, it is convenient to observe the crossover from nucleation to a coalescence regime, within shorter period (simulational time scale). Numerically, we found that the logarithm of the nucleation time is proportional to the inverse field ($1/h$) which is consistent with the results obtained from CNT (eqn (1)). The slopes are also been estimated numerically. The slope in the nucleation regime is nearly 0.79 and that in the coalescence regime is approximately 0.27, which is roughly 1/3 of that in the nucleation regime. This is consistent with the results from CNT. We know [6]

$$a\sigma(T)/KT_c = -2(T/T_c - 1)\log_e(\sqrt{2} + 1)$$

where a is the lattice separation ($a = 1$, here). In the above formula, putting $J/KT = 5/8$, we get

$$\pi\sigma^2(T)/T = 2.733.$$

So, according to CNT,

$$\tau \sim \exp(2.733/h) \sim 10^{(1.187/h)}.$$

So, the slope (at $J/KT = 5/8$) in the nucleation regime, is estimated to be equal to 1.187 [6]. However, the simulation results give 0.79. This mismatch may be due to the nonspherical shape of the droplets (assumed in CNT). It would be worth mentioning here that the theoretically calculated [6] slope (using the diagonal interface tension) at the temperature used is 1.900.

We have also studied the variation of the crossover field (h_c ; at which the crossover from nucleation regime to a coalescence regime starts) and the crossover time (τ_c ; the nucleation time at the crossover point) with the system size. From CNT, the nucleation time and the field is related as

$$\tau \sim \frac{1}{J \times L^2} \sim \exp(\pi\sigma^2/hKT)/L^2$$

At the crossover point (τ_c, h_c)

$$\tau_c \sim \exp(\pi\sigma^2/h_cKT)/L^2.$$

If we assume $\tau_c \sim L^2$, then

$$h_c \sim 1/\log(L). \quad (3)$$

Figure 2 shows that plot of crossover field (h_c) versus $1/\log(L)$ and it is indeed a straight line, which is consistent with the results of CNT (eqn (3)). Figure 3 shows the variation of crossover time (τ_c) with respect to L^2 , which is a straight line. This also proves that the assumption $\tau_c \sim L^2$ is correct in the derivation of equation (3).

IV. Summary

We have studied the nucleation in the two dimensional Ising system by Monte Carlo simulation with heat-bath dynamics. The logarithm of the nucleation time is found to be proportional to the inverse magnetic field. The proportionality constant (related with the surface tension) has been estimated and found to be close to that calculated from CNT. The nucleation time has been studied for various system sizes which shows a crossover from the nucleation regime to a coalescence regime. The crossover field is found to be proportional to the inverse of the logarithm of the system size and the crossover time is found to be proportional to the square of the system size. The results are consistent with the prediction of classical nucleation theory.

Acknowledgements: Sonderforschungsbereich 341 is gratefully acknowledged for financial support. Author would like to thank D. Stauffer for suggesting the problem and useful comments.

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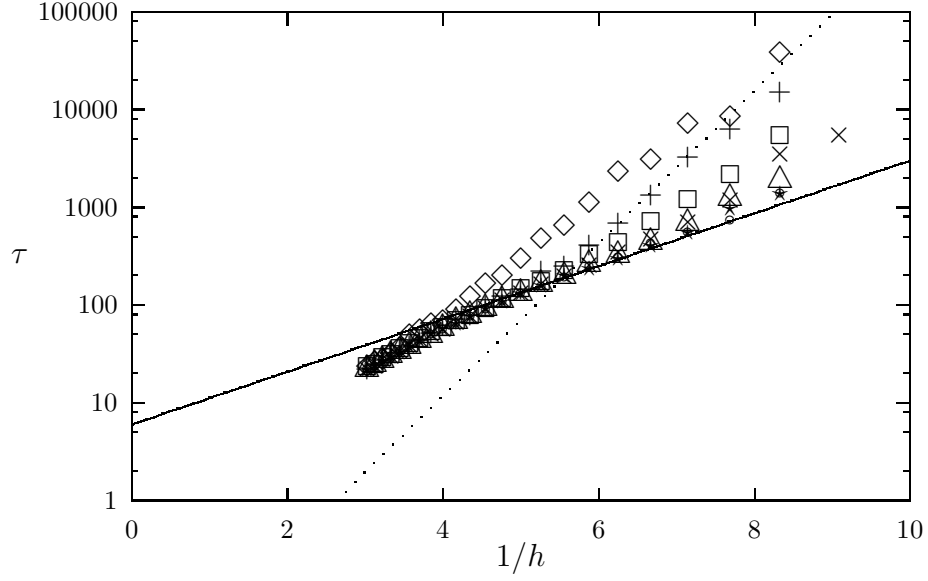


Fig. 1. Nucleation time (τ) is plotted against the inverse field ($1/h$) for various system sizes. (\diamond) $L = 51$, ($+$) $L = 101$, (\square) $L = 151$, (\times) $L = 201$, (\triangle) $L = 251$, (\star) $L = 351$ and (\circ) $L = 401$. $J/KT = 5/8$ here. The two straight lines are the best fitted straight lines in the coalescence and nucleation regimes.

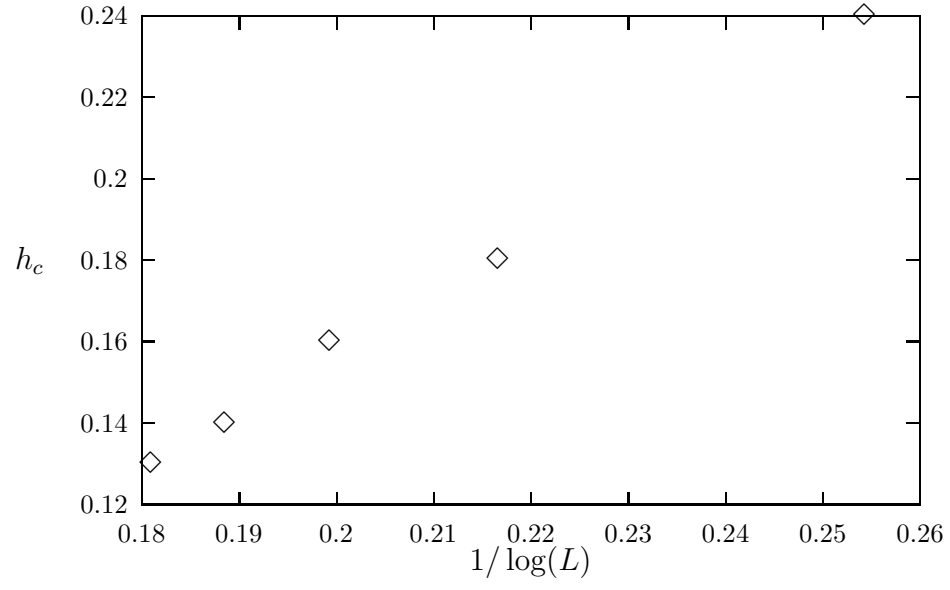


Fig.2. The crossover field (h_c) is plotted against $1/\log(L)$.

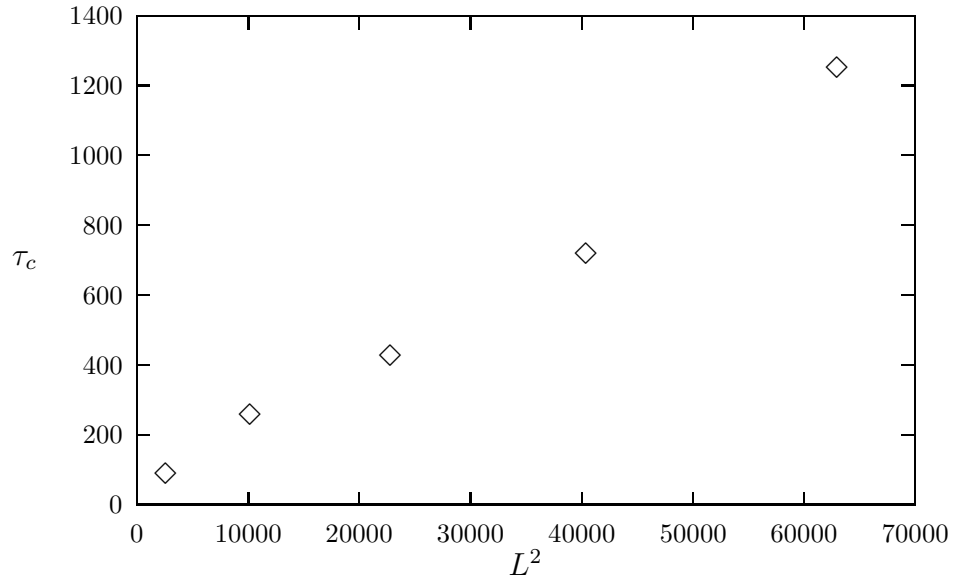


Fig. 3. The crossover time (τ_c) is plotted against L^2 .